

Slow in-plane magnetoresistance oscillations in multiband quasi-two-dimensional metals

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Received: date / Accepted: date

Abstract Slow oscillations (SIO) of magnetoresistance is a convenient tool to measure electronic structure parameters in quasi-two-dimensional metals. We study the possibility to apply this method to multi-band conductors, e.g. to iron-based high-temperature superconducting materials. We show that SIO can be used to measure the interlayer transfer integral in multi-band conductors similar to single-band metals. In addition, the SIO allow to measure and compare the effective masses or the electron scattering rates in various bands.

Keywords Fermi surface · Quantum oscillations · Fe-based superconductors · Slow oscillations · Magnetoresistance

1 Introduction

Discovery of the superconductivity in iron-based materials [1] raised a question about the nature of the underlying electron pairing. Most promising is the electronic mechanism of Cooper pair formation originating from

the dominating exchange of either spin or orbital fluctuations [2,3]. Former results in the extended s -wave order parameter that change sign between electron and hole Fermi surface pockets, the so-called s_{\pm} state [3,4,5,6,7]. Orbital fluctuations enhanced by the electron-phonon coupling may lead to the sign-preserving s -wave gap, the s_{++} state [8,9].

Since electronic mechanisms of pairing involves particles near the Fermi level, knowledge of the topology and details of the Fermi surface (FS) is crucial. There are several experimental methods of determining it. Widely used are angle-resolved photoemission spectroscopy (ARPES) and magnetic quantum oscillations (MQO) measurements. ARPES provides a lot of valuable information on the electronic structure [10,11] especially considering the quasi-two-dimensional nature of Fe-based materials, but its surface sensitivity sometime may be a severe limitation. In this respect, MQO are more reliable method of determining the bulk properties. MQO measurements were performed on a number of Fe-based materials, both pnictides and chalcogenides [12]. In particular, data are available for LaFePO [13,14], undoped 122 systems [15,16,17,18,19], BaFe₂(As_{1-x}P_x)₂ [20,21], KFe₂As₂ [22], 111 systems LiFeP and LiFeAs [23], and 11 system FeSe [24].

The iron-based superconducting materials, as well as most other high- T_c superconductors, have a strong quasi-two-dimensional (Q2D) anisotropy of electronic dispersion and conductivity. In the tight-binding approximation the electronic dispersion of Q2D metals is given by

$$\epsilon_{3D}(\mathbf{k}) \approx \sum_{\eta} \epsilon_{\eta}(\mathbf{k}_{||}) - 2t_{z,\eta}(\mathbf{k}_{||}) \cos(k_z d), \quad (1)$$

where η numerates different Fermi-surface pockets (or bands) with in-plane dispersion $\epsilon_{\eta}(\mathbf{k}_{||})$, $\mathbf{k}_{||} = \{k_x, k_y\}$

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is the in-plane electron momentum, d is the interlayer lattice constant, and the interlayer transfer integral t_z is much less than the in-plane Fermi energy $E_{F\eta} = \mu_\eta$ of any band η . Below we assume that t_z is momentum-independent and the same for all bands η : $t_{z,\eta}(\mathbf{k}_{||}) = t_z$. Then the Fermi surface of each band is a cylinder with weak warping $\sim 4t_z/E_F \ll 1$. The MQO with such FS have two close fundamental frequencies $F_0 \pm \Delta F$. In a magnetic field $\mathbf{B} = B_z$ perpendicular to the conducting layers $F_0/B = \mu_\eta/\hbar\omega_{c,\eta}$ and $\Delta F/B = 2t_z/\hbar\omega_{c,\eta}$, where $\hbar\omega_{c,\eta} = \hbar eB_z/m_\eta^*c$ is the distance between the Landau levels (LL), sometimes called the cyclotron energy, and m_η^* is an effective electron mass for this band η .

Magnetoresistance (MR) in layered Q2D conductors has interesting features, which do not appear in 3D metals. At $2t_z < \mu$ the angular oscillations of interlayer MR (AMRO) have been observed in many layered organic metals (see, e.g., Refs. [26,27,28,29] for reviews) and in some cuprate high- T_c superconductors [30], which was interpreted as a signature of a well-defined quasi-2D Fermi surface in these materials. For an isotropic in-plane electron dispersion AMRO are qualitatively described by the renormalization of the interlayer transfer integral:[31]

$$t_z = t_z(\theta) = t_z(0) J_0(k_F d \tan \theta), \quad (2)$$

where $J_0(x)$ is the Bessel's function, $p_F = \hbar k_F$ is the in-plane Fermi momentum, and θ is the angle between the magnetic field \mathbf{B} and the normal to conducting layers.

At $t_z \sim \hbar\omega_c$ several additional qualitative features of MR appear. For example, the strong monotonic growth of interlayer MR $R_{zz}(B_z)$ was observed in various Q2D metals [32,33,34,35,36,37,38,39,44,40] and recently theoretically explained [40,41,42,43]. At $t_z \gtrsim \hbar\omega_c$ the MR acquires the so-called slow oscillations [44,45] and the phase shift of beats [46,45]. These two effects appear in the higher orders in $\hbar\omega_c/t_z$ and, therefore, are missed in the standard 3D theory of MR [47,48,49].

These slow oscillations (SIO) originate from the finite interlayer hopping t_z contrary to usual MQO with low frequency, originating from small FS pockets. The product of oscillations with two close frequencies $F_0 \pm \Delta F$ gives oscillations with frequency $2\Delta F$:

$$\cos(F_0 + \Delta F) \cos(F_0 - \Delta F) = \frac{\cos(2F_0) + \cos(2\Delta F)}{2}. \quad (3)$$

The conductivity, being a non-linear function of the oscillating electronic density of states (DoS) and of the diffusion coefficient, has SIO with frequency $2\Delta F \propto t_z$, while the magnetization, being a linear functional of DoS, does not show SIO [44,45]. The SIO have many

interesting and useful features as compared to the quantum oscillations. First, they survive at much higher temperature than MQO, because, contrary to MQO, they are not suppressed by the temperature smearing of Fermi distribution function. Second, they are not sensitive to a long-range disorder, which damps the fast MQO similarly to finite temperature due to a spatial variation of the Fermi energy. Third, the SIO allow to measure the interlayer transfer integral t_z and the in-plane Fermi momentum $p_F \equiv \hbar k_F$. These features make the SIO to be a useful tool to study the electronic properties of Q2D metals. Almost 30 years since their discovery [50] and more than 10 years after their explanation [44,45] the SIO were investigated only for the *interlayer* conductivity $\sigma_{zz}(B)$, when the current and the magnetic field are both applied perpendicularly to the 2D layers, and only in organic compounds. The SIO were shown to be a useful and very accurate tool to measure the interlayer transfer integral t_z . In addition, the SIO allow to obtain information about the in-plane Fermi momentum k_F and even about the type of disorder, as short- or long-range disorder [44,45]. Later it was realized that the monocrystals of most layered Q2D compounds, including pnictide high-temperature superconductors, as a rule, have the shape of very thin flakes for which the correct measurements of the interlayer conductivity is very difficult, especially in the case of good metallic properties of studied compounds. Recently, the first measurements and qualitative analysis of SIO of the intralayer (in-plane) conductivity in the non-organic layered Q2D rare-earth tritelluride compounds $R\text{Te}_3$ ($R = \text{Gd}$ and Tb) was reported [51]. From these experimental data for the first time in these strongly anisotropic Q2D conductors the authors obtained the value of the interlayer transfer integral t_z and estimated the in-plane Fermi momentum after the FS reconstruction due to the double charge-density-wave superstructure [51]. Thus, the slow oscillations of MR proved to be a powerful technique to explore the electronic structure of various compounds. In this report we investigate the possibility of its application to the multiband systems like iron-based high- T_c superconducting materials.

Contrary to the situation in the strongly correlated high- T_c cuprates, consensus between electronic band structure calculations in the density functional theory (DFT), ARPES, QO, and Compton scattering [25] has been promptly established, so that the in-plane electron dispersion $\epsilon_\eta(\mathbf{k}_{||})$ for each band η is known. The gross feature is that excluding the cases of extreme hole and electron dopings, the in-plane FS in Fe-based materials consists of two or three hole pockets around the $\Gamma = (0,0)$ point and two electron pockets around the

$M = (\pi, \pi)$ point in the 2-Fe Brillouin zone corresponding to the crystallographic unit cell. The scattering between these two groups of FSs believed to be responsible for the stripe antiferromagnetic order in undoped materials and for the spin fluctuation mediated pairing in doped compounds. Thus the two-band model is the minimal model capturing the basic yet essential physics of pnictides and chalcogenides (see discussion in Ref. [3]). Below we generalize the qualitative study of SIO of intralayer MR in Ref. [51] from the one-band to a multi-band model, assuming that there are λ different bands.

2 Calculations

According to Eq. (90.5) of Ref. [52] the intralayer conductivity at finite temperature is given by [52]

$$\sigma_{yy} = \int d\varepsilon [-n'_F(\varepsilon)] \sigma_{yy}(\varepsilon), \quad (4)$$

where the derivative of the Fermi distribution function $n'_F(\varepsilon) = -1/\{4T \cosh^2[(\varepsilon - \mu)/2T]\}$, and the zero-temperature electron conductivity at energy ε is

$$\sigma_{yy}(\varepsilon) = \sum_{\eta} \sigma_{yy,\eta}(\varepsilon) = \sum_{\eta} e^2 g_{\eta}(\varepsilon) D_{y,\eta}(\varepsilon). \quad (5)$$

Here $g_{\eta}(\varepsilon)$ is the DoS and $D_{y,\eta}(\varepsilon)$ is the diffusion coefficient along y-axis of electrons from the band η . It is convenient to use the harmonic expansion for the oscillating DoS $g_{\eta}(\varepsilon)$. Below we will need only the first terms in this harmonic series, which at finite $t_z \sim \hbar\omega_c$ are given by [54, 55, 45]

$$g_{\eta}(\varepsilon) \approx g_{0,\eta} \left[1 - 2 \cos \left(\frac{2\pi\varepsilon}{\hbar\omega_{c,\eta}} \right) J_0 \left(\frac{4\pi t_z}{\hbar\omega_{c,\eta}} \right) R_{D,\eta} \right], \quad (6)$$

where $g_{0,\eta} = m_{\eta}^*/\pi\hbar^2 d$ is the DoS per two spin components at the Fermi level from the band η in the absence of magnetic field, $J_0(x)$ is the Bessel's function, $R_{D,\eta} \approx \exp[-\pi/\omega_{c,\eta}\tau_{0,\eta}]$ is the Dingle factor [59, 60], $\tau_{0,\eta}$ is the electron mean free time without magnetic field, which for scattering by point-like impurities depends only on the total DoS and not on the band index η : $\tau_{0,\eta} = \tau_0 = \hbar/2\Gamma_0$, where Γ_0 is the LL broadening.

The calculation of the diffusion coefficient $D_y(\varepsilon)$ is less trivial and requires to specify the model. At $\mu \gg \hbar\omega_c$ the quasi-classical approximation is applicable. In an ideal crystal in a magnetic field \mathbf{B} the electrons move along the cyclotron orbits with a fixed center and the Larmor radius of band η , $R_{L,\eta} = p_{F,\eta}c/eB_z$. Without scattering the electron diffusion in the direction perpendicular to \mathbf{B} is absent. The electron-electron

(e-e) interaction in the absence of magnetic field and of umklapp processes does not change the total electron momentum and, hence, does not change electric conductivity, though in combination with disorder, the e-e interaction leads to substantial corrections to conductivity [61]. Scattering by impurities changes the electronic states and leads to the electron diffusion perpendicular to magnetic field, and we take into account only this mechanism of the in-plane electron diffusion in perpendicular magnetic field. For simplicity, we consider only the scattering by short-range impurities, described by the δ -function potential: $V_i(r) = U\delta^3(r - r_i)$. Scattering by impurities is elastic, i.e. it conserves the electron energy ε , but the quantum numbers of electron states may change. The matrix element of impurity scattering is given by

$$T_{mm'} = \Psi_{m'}^*(r_i) U \Psi_m(r_i), \quad (7)$$

where $\Psi_m(r)$ is the electron wave function in the state m . During each scattering, the typical change $\Delta y = \Delta P_x c/eB_z$ of the mean electron coordinate y_0 perpendicular to \mathbf{B} is of the order of $R_{L,\eta}$, because for larger $\Delta y \gg R_L$ the matrix element in Eq. (7) is exponentially small because of small overlap of the electron wave functions $\Psi_{m'}^*(r_i) \Psi_m(r_i) \sim \Psi_m^*(r_i + \Delta y) \Psi_m(r_i)$ [56]. The diffusion coefficient for the band η is approximately given by

$$D_{y,\eta}(\varepsilon) \approx \langle (\Delta y)^2 \rangle_{\eta} / 2\tau_{\eta}(\varepsilon), \quad (8)$$

where $\tau_{\eta}(\varepsilon)$ is the energy-dependent electron mean scattering time by impurities, and the angular brackets in Eq. (8) mean averaging over impurity scattering events. In the Born approximation, the mean scattering rate on point-like impurities is independent on the band η and given by

$$1/\tau_{\eta}(\varepsilon) = 1/\tau(\varepsilon) = 2\pi n_i U^2 g(\varepsilon), \quad (9)$$

where n_i is the impurity concentration and $g(\varepsilon) \equiv \sum_{\eta} g_{\eta}(\varepsilon)$ is the total DoS. This scattering rate has MQO, which are reduced as compared to those of the DoS in Eq. (6), because MQO of the DoS from different bands have different frequencies and partially cancel each other. Indeed, if one takes the total number of bands $\lambda > 1$ and the same average DoS from each band: $g_{0,\eta} = g_0$, one obtains

$$\frac{g(\varepsilon)}{\lambda g_0} \approx 1 - \sum_{\eta} \frac{2}{\lambda} \cos \left(\frac{2\pi\varepsilon}{\hbar\omega_{c,\eta}} \right) J_0 \left(\frac{4\pi t_z}{\hbar\omega_{c,\eta}} \right) R_{D,\eta}. \quad (10)$$

The MQO of $\langle (\Delta y)^2 \rangle_{\eta} \approx R_{L,\eta}^2$ are, usually, weaker than MQO of $g_{\eta}(\varepsilon)$, and in 3D metals they are neglected [52]. Then

$$D_{y,\eta}(\varepsilon) \approx R_{L,\eta}^2 / 2\tau(\varepsilon) \propto g(\varepsilon). \quad (11)$$

However, in Q2D metals, when $t_z \sim \hbar\omega_c$, the MQO of $\langle(\Delta y)^2\rangle$ can be of the same order as MQO of the DoS. Moreover, they are not suppressed as strongly by the averaging over various bands η , as $g(\varepsilon)$ is. Therefore, instead of Eq. (11) at $R_D \ll 1$ one has

$$\frac{D_{y,\eta}(\varepsilon)}{D_{0,\eta}} \approx 1 - 2\alpha_\eta \cos\left(\frac{2\pi\varepsilon}{\hbar\omega_{c,\eta}}\right) J_0\left(\frac{4\pi t_z}{\hbar\omega_{c,\eta}}\right) R_{D,\eta} \quad (12)$$

$$- \sum_{\eta' \neq \eta} 2\beta_{\eta\eta'} \cos\left(\frac{2\pi\varepsilon}{\hbar\omega_{c,\eta'}}\right) J_0\left(\frac{4\pi t_z}{\hbar\omega_{c,\eta'}}\right) R_{D,\eta'},$$

where $D_{0,\eta} \approx R_{L,\eta}^2/2\tau_\eta$, and the numbers $\alpha_\eta \sim 1$ and $\beta_{\eta\eta'} \sim 1/\lambda$. Combining Eqs. (5), (6) and (12) one obtains

$$\sigma_{yy}(\varepsilon) = e^2 \sum_{\eta} g_{0,\eta} D_{0,\eta} \times \quad (13)$$

$$\times \left[1 - 2\cos\left(\frac{2\pi\varepsilon}{\hbar\omega_{c,\eta}}\right) J_0\left(\frac{4\pi t_z}{\hbar\omega_{c,\eta}}\right) R_{D,\eta} \right]$$

$$\times \left[1 - 2\alpha_\eta \cos\left(\frac{2\pi\varepsilon}{\hbar\omega_{c,\eta}}\right) J_0\left(\frac{4\pi t_z}{\hbar\omega_{c,\eta}}\right) R_{D,\eta} \right.$$

$$\left. - \sum_{\eta' \neq \eta} 2\beta_{\eta\eta'} \cos\left(\frac{2\pi\varepsilon}{\hbar\omega_{c,\eta'}}\right) J_0\left(\frac{4\pi t_z}{\hbar\omega_{c,\eta'}}\right) R_{D,\eta'} \right].$$

The slow oscillations arise from the product of second terms in both square brackets with the same cyclotron frequency $\omega_{c,\eta} = \omega_{c,\eta'}$, i.e. $\eta = \eta'$, because only these terms give the energy-independent term $1/2$, which is not affected by the averaging over ε : $\cos^2(2\pi\varepsilon/\hbar\omega_{c,\eta}) = [1 + \cos(4\pi\varepsilon/\hbar\omega_{c,\eta})]/2$. Hence, the classical (monotonic + slow oscillating) part of $\sigma_{yy}(B)$ is obtained by collecting all leading energy independent terms in Eq. (4) with subsequent trivial integration over ε after substitution to Eq. (4),

$$\sigma_{yy}^{SIO}(B) \approx e^2 \sum_{\eta} g_{0,\eta} D_{0,\eta} \left[1 + 2\alpha_\eta J_0^2\left(\frac{4\pi t_z}{\hbar\omega_{c,\eta}}\right) R_{D,\eta}^2 \right]. \quad (14)$$

The other cross products in Eq. (13) give MQO, i.e. the ε -dependent terms $\propto \cos(2\pi\varepsilon/\hbar\omega_{c,\eta'})$, which after temperature smearing in Eq. (4) acquire the usual temperature damping factor of MQO:

$$R_{T,\eta} = (2\pi^2 k_B T / \hbar\omega_{c,\eta}) / \sinh(2\pi^2 k_B T / \hbar\omega_{c,\eta}). \quad (15)$$

On contrary, the SIO in Eq. (14) are not damped by temperature within our model.

Approximately, one can use the asymptotic expansion of the Bessel function in Eq. (14) for large values of the argument: $J_0(x) \approx \sqrt{2/\pi x} \cos(x - \pi/4)$, $x \gg 1$. Then, after introducing the frequencies of SIO,

$$F_{SIO,\eta} = 4t_z B / \hbar\omega_{c,\eta}, \quad (16)$$

Eq. (14) simplifies to

$$\sigma_{yy}^{SIO}(B) \approx e^2 \sum_{\eta} g_{0,\eta} D_{0,\eta} \times \quad (17)$$

$$\times \left[1 + \frac{\alpha \hbar\omega_{c,\eta}}{2\pi^2 t_z} \sin\left(\frac{2\pi F_{SIO,\eta}}{B}\right) R_{D,\eta}^2 \right].$$

In tilted magnetic field at constant $|\mathbf{B}|$, $\omega_c \propto \cos\theta$ and t_z changes according to Eq. (2). Then the frequencies of SIO will depend on tilt angle θ of magnetic field (with respect to the normal to conducting layers) as

$$F_{SIO,\eta}(\theta) / F_{SIO,\eta}(0) = J_0(k_{F,\eta} d \tan\theta) / \cos(\theta). \quad (18)$$

Note that this dependence is non-monotonic and crucially different from the angular dependence of MQO frequencies, given by the simple cosine law: $F_{MQO}(\theta) / F_{MQO}(0) = 1/\cos(\theta)$.

3 Discussion and conclusions

As one can see by comparing Eq. (17) with the results of Ref. [51], for multiband conductors both the slow oscillations and MQO of magnetoresistance are damped in their relative amplitude by the factor $\sim 1/\lambda$ as compared to single-band conductors, where λ is the number of different bands. The origin is the different contributions to the sum over η from the first (unity) and the second (band-dependent) terms in the square brackets. This is similar to the relative damping of the MQO of the DoS in Eq. (10). Nevertheless, the SIO can be observed and used to extract the parameters of electronic structure from experimental data.

As one can see from Eq. (17), the slow oscillations of MR in multi-band conductors are in most aspects similar to SIO in single-band conductors, studied in Refs. [44,45,51]. Each frequency of SIO corresponds to a particular band η and can be used to extract electronic parameters of this band. For the case of in-plane momentum-independent interlayer hopping t_z , if the cyclotron mass or Landau-level separation is known for at least one band, i.e. from the temperature dependence of MQO amplitude, the frequency $F_{SIO,\eta}$ of slow oscillations of magnetoresistance for this band gives the value of the interlayer transfer integral t_z according to Eq. (16). The angular dependence of the SIO frequency has a non-monotonic angular dependence given by Eq. (18), which allows to extract the Fermi momentum $k_{F,\eta}$ for this particular band as function of the azimuth angle ϕ from experimental data on SIO. Since the interlayer transfer integral is the same for all bands, the measured ratios of the SIO frequencies for various bands η give the ratios of their effective (cyclotron) masses m_η^* , which allows to determine m_η^* for

all bands if m_η^* is known for at least one band. This application of SIO was absent for single-band metals, being new for the multi-band conductors. This application is very helpful, because the temperature dependence of the MQO amplitudes cannot always be clearly fitted by the Lifshitz-Kosevich formula and by Eq. (15) for all observed frequencies. If there is an independent way to determine t_z , the SIO give an alternative way to determine all effective masses m_η^* . The damping of slow oscillations, determined only by the Dingle factor, can be used to compare the Dingle temperatures and, therefore, the scattering amplitudes for different bands.

To summarize, in this paper we have shown the possibility of using rather new phenomenon, namely, the slow oscillations of magnetoresistance, to measure the parameters of electronic structure of multi-band quasi-two-dimensional conductors. The application of this method to multi-band conductors has some specific features, absent for single-band metals, which allow to extract and compare the electronic parameters of different bands. We believe, that this technique can be used to measure the interlayer transfer integral t_z and other important parameters in iron-based pnictides and chalcogenides, MgB_2 , Sr_2RuO_4 , and in a variety of multiband conductors and superconductors.

Acknowledgements We are grateful to V.M. Pudalov, I.A. Nekrasov and S.G. Ovchinnikov for useful discussions. We acknowledge the partial support by RFBR (Grants 13-02-01395 and 13-02-00178) and the President Grant for Government Support of the Leading Scientific Schools of the Russian Federation (NSh-2886.2014.2).

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